

# Equation of state near the endpoint of the critical line

S. SEIDE

and

C. WETTERICH\*

*Institut für Theoretische Physik  
Universität Heidelberg  
Philosophenweg 16  
69120 Heidelberg, Germany*

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## Abstract

We discuss first order transitions for systems in the Ising universality class. The critical long distance physics near the endpoint of the critical line is explicitly connected to microscopic properties of a given system. Information about the short distance physics can therefore be extracted from the precise location of the endpoint and non-universal amplitudes. Our method is based on non-perturbative flow equations and yields directly the universal features of the equation of state, without additional theoretical assumptions of scaling or resummations of perturbative series. The universal results compare well with other methods.

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\*Email: C.Wetterich@thphys.uni-heidelberg.de

# 1 Introduction

Many phase transitions are described near the critical temperature by a one-component scalar field theory without internal symmetries. A typical example is the water-vapour transition where the field  $\varphi(x)$  corresponds to the average density field  $n(x)$ . At normal pressure one observes a first order transition corresponding to a jump in  $\varphi$  from high (water) to low (vapour) values as the temperature  $T$  is increased. With increasing pressure the first order transition line ends at some critical pressure  $p_*$  in an endpoint. For  $p > p_*$  the phase transition is replaced by an analytical crossover.

This behaviour is common to many systems and characterizes the universality class of the Ising model. As another example from particle physics, the high temperature electroweak phase transition in the early universe is described by this universality class if the mass of the Higgs particle in the standard model is near the endpoint value  $M_{H*} \approx 72\text{GeV}$ [1]. An Ising type endpoint should also exist if the high temperature or high density chiral phase transition in QCD or the gas-liquid transition for nuclear matter are of first order in some region of parameter space.

Very often the location of the endpoint - e.g. the critical  $T_*$ ,  $p_*$  and  $n_*$  for the liquid-gas transition - is measured quite precisely. The approach to criticality is governed by universal scaling laws with critical exponents. Experimental information is also available about the non-universal amplitudes appearing in this scaling behaviour. These non-universal critical properties are specific for a given system, and the question arises how they can be used to gain precise information about the underlying microscopic physics. This problem clearly involves the difficult task of an explicit connection between the short distance physics and the collective behaviour leading to a very large correlation length.

So far renormalization group methods [2, 3, 4] have established the structure of this relation and led to a precise determination of the universal critical properties. A suitable implementation of these ideas should allow us to complete the task by mapping details of microscopic physics to non-universal critical quantities. In this paper we show that this is indeed possible. A demonstration is given for the liquid-gas transition in carbon dioxide.

A very useful concept for the study of phase transitions is the coarse grained free energy or effective average action  $\Gamma_k[\varphi]$  [5, 6]. It is related to the (grand canonical) partition function in presence of an effective infrared cutoff  $R_k$ ,

$$Z_k[j] = \int \mathcal{D}\chi \exp \left\{ -S[\chi] + \int d^3x \left( j(x)\chi(x) - \frac{1}{2}\chi(x)R_k(-\partial^2)\chi(x) \right) \right\}, \quad (1.1)$$

by a Legendre transform:

$$\begin{aligned} \Gamma_k[\varphi] &= -\ln Z_k[j] + \int d^3x \left( j(x)\varphi(x) - \frac{1}{2}\varphi(x)R_k(-\partial^2)\varphi(x) \right) \\ \varphi(x) &= \frac{\delta}{\delta j(x)} \ln Z_k[j]. \end{aligned} \quad (1.2)$$

For the liquid-gas transition  $\chi(x)$  is the microscopic density field,  $S[\chi] = H/T$  the microscopic or classical action and  $j(x)$  the source, which will be specified below. The

momentum dependent infrared cutoff obeys  $R_k(q^2) \sim k^2$  for  $q^2 \ll k^2$  and should vanish rapidly for  $q^2 \gg k^2$ . This assures that only fluctuations with momenta  $q^2 > k^2$  are effectively included in the functional integral (1.1). Below, we will often not consider the most general form of  $\Gamma_k$  but rather work with a truncation which only includes the most general terms containing up to two derivatives,

$$\Gamma_k[\varphi] = \int d^3x \left\{ U_k(\varphi(x)) + \frac{1}{2} Z_k(\varphi(x)) \partial^\mu \varphi \partial_\mu \varphi \right\}. \quad (1.3)$$

Our final aim will be the computation of the potential  $U \equiv U_{k \rightarrow 0}$  and the wave function renormalization  $Z \equiv Z_{k \rightarrow 0}$  for a vanishing (or very small) infrared cutoff. In absence of the infrared cutoff the shape of  $U(\varphi)$  directly determines the equation of state. For a homogeneous situation  $UT$  corresponds to the free energy density. Indeed, expressing  $U$  as a function of the density one finds for the liquid-gas system at a given chemical potential  $\mu$

$$\frac{\partial U}{\partial n} = \frac{\mu}{T}. \quad (1.4)$$

Equivalently, one may also use the more familiar form of the equation of state in terms of the pressure  $p$ ,

$$n^2 \frac{\partial}{\partial n} \left( \frac{U}{n} \right) = \frac{p}{T}. \quad (1.5)$$

(Here the additive constant in  $U$  is fixed such that  $U(n=0)=0$ ). The wave function renormalization  $Z(\varphi)$  contains the additional information needed for the two point correlation function at large distance for arbitrary pressure.

A direct computation of  $U(\varphi)$  and  $Z(\varphi)$  becomes, however, a difficult problem for all situations where the correlation length becomes large and collective phenomena are therefore important. For the water-vapour transition this happens in the vicinity of the endpoint, i.e. for a pressure and temperature near  $p_*$  and  $T_*$ . In this case the free energy can best be calculated by a stepwise procedure where  $k$  is lowered consecutively. One starts at some large  $k$  where only short distance fluctuations are included and a relatively simple microphysical computation is reliable. As  $k$  is lowered, the effects of fluctuations with longer wavelengths are added. We will describe the dependence of the average action on  $k$  by a non-perturbative flow equation which can be derived from an exact renormalization group equation.

In this way the computation of thermodynamic potentials, correlation length etc. is done in two steps: The first is the computation of a short distance free energy  $\Gamma_\Lambda$ . This does not involve large length scales and can be done by a variety of expansion methods or numerical simulations. This step is not the main emphasis of the present paper and we will use a relatively crude approximation for the gas-liquid transition. The second step is more difficult and will be addressed here. It involves the relation between  $\Gamma_\Lambda$  and  $\Gamma_0$ , and has to account for possible complicated collective long distance fluctuations.

For a large infrared cutoff  $k = \Lambda$  one may compute  $\Gamma_\Lambda$  perturbatively. For example,

the lowest order in a virial expansion for the liquid-gas system yields

$$U_\Lambda(n) = -n \left( 1 + \ln g + \frac{3}{2} \ln \frac{MT}{2\pi\Lambda^2} \right) + n \ln \left( \frac{n}{(1 - b_0(\Lambda)n)\Lambda^3} \right) - \frac{b_1(\Lambda)}{T} n^2 + c_\Lambda. \quad (1.6)$$

Here  $\Lambda^{-1}$  should be of the order of a typical range of intermolecular interactions,  $M$  and  $g$  are the mass and the number of degrees of freedom of a molecule and  $b_0, b_1$  parameterize the virial coefficient  $B_2(T) = b_0 - b_1/T$ .<sup>1</sup> (The (mass) density  $\rho$  is related to the particle density  $n$  by  $\rho = Mn$ .) We emphasize that the convergence of a virial expansion is expected to improve considerably in presence of an infrared cutoff  $\Lambda$  which suppresses the long distance fluctuations.

The field  $\varphi(x)$  is related to the (space-dependent) particle density  $n(x)$  by

$$\varphi(x) = K_\Lambda(n(x) - \hat{n}) \quad (1.7)$$

with  $\hat{n}$  some suitable fixed reference density. We approximate the wave function renormalization  $Z_\Lambda$  by a constant. It can be inferred from the correlation length  $\hat{\xi}$ , evaluated at some reference density  $\hat{n}$  and temperature  $\hat{T}$  away from the critical region, through

$$\hat{\xi}^{-2} = Z_\Lambda^{-1} \frac{\partial^2 U}{\partial \varphi^2} \big|_{\hat{\varphi}, \hat{T}}. \quad (1.8)$$

For a suitable scaling factor

$$K_\Lambda = \left( \frac{1}{\hat{n}} + \frac{b_0(2 - b_0\hat{n})}{(1 - b_0\hat{n})^2} - \frac{2b_1}{\hat{T}} \right)^{1/2} \hat{\xi} \quad (1.9)$$

one has  $Z_\Lambda = 1$ .

We observe that the terms linear in  $n$  in eq. (1.6) play only a role for the relation between  $n$  and  $\mu$ . It is instructive to subtract from  $U_\Lambda$  the linear piece in  $\varphi$  and to expand in powers of  $\varphi$ :

$$U_\Lambda(\varphi) = \frac{m_\Lambda^2}{2} \varphi^2 + \frac{\gamma_\Lambda}{6} \varphi^3 + \frac{\lambda_\Lambda}{8} \varphi^4 + \dots \quad (1.10)$$

with

$$\begin{aligned} m_\Lambda^2 &= K_\Lambda^{-2} \left( \frac{1}{\hat{n}} + \frac{b_0(2 - b_0\hat{n})}{(1 - b_0\hat{n})^2} - \frac{2b_1}{\hat{T}} \right) \\ \gamma_\Lambda &= K_\Lambda^{-3} \left( \frac{b_0^2(3 - b_0\hat{n})}{(1 - b_0\hat{n})^3} - \frac{1}{\hat{n}^2} \right) \\ \lambda_\Lambda &= \frac{2}{3} K_\Lambda^{-4} \left( \frac{b_0^3(4 - b_0\hat{n})}{(1 - b_0\hat{n})^4} + \frac{1}{\hat{n}^3} \right). \end{aligned} \quad (1.11)$$

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<sup>1</sup> The Van der Waals coefficients  $b_0, b_1$  for real gases can be found in the literature. These values are valid for small densities. They also correspond to  $k = 0$  rather than to  $k = \Lambda$ . Fluctuation effects lead to slightly different values for  $b_i(\Lambda)$  and  $b_i(k = 0)$  even away from the critical line. We find that these differences are small for  $n \ll n_*$ . Similarly, a constant  $c_\Lambda$  should be added to  $U_\Lambda$  such that  $U_0(0) = 0$ .

For a convenient choice  $\hat{n} = \frac{1}{3b_0}$ ,  $\hat{T} = \frac{8}{11} \frac{b_1}{b_0}$  one has  $\gamma_\Lambda = 0$  and

$$K_\Lambda = 2b_0^{1/2}\hat{\xi}, \quad m_\Lambda^2 = \left(\frac{27}{16} - \frac{b_1}{2b_0T}\right)\hat{\xi}^{-2}, \quad \lambda_\Lambda = \frac{243}{128}b_0\hat{\xi}^{-4}. \quad (1.12)$$

Typical values for carbon dioxide at the endpoint are  $m_\Lambda^2/\Lambda^2 = -0.31$ ,  $\lambda_\Lambda/\Lambda = 6.63$  for  $\Lambda^{-1} = 5 \cdot 10^{-10} \text{ m}$ ,  $\hat{\xi} = 0.6 \Lambda^{-1}$ . In the limit (1.10) one obtains a  $\varphi^4$ -model. Our explicit calculations for carbon dioxide will be performed, however, for the microscopic free energy (1.6). The linear piece in the potential can be absorbed in the source term such that the equation of state reads <sup>2</sup>

$$\frac{\partial U}{\partial \varphi} = j, \quad j = K_\Lambda^{-1} \left( \frac{\mu}{T} + 1 + \ln g + \frac{3}{2} \ln \frac{MT}{2\pi\Lambda^2} \right). \quad (1.13)$$

We emphasize that a polynomial microscopic potential (1.10) with equation of state  $\partial U/\partial \varphi = j$  is a good approximation for a large variety of different systems. For the example of magnets  $\varphi$  corresponds to the magnetization and  $jT$  to the external magnetic field. For  $\gamma_\Lambda = 0$  and  $\lambda_\Lambda \rightarrow \infty$ , with finite negative  $m_\Lambda^2/\lambda_\Lambda$ , this is the  $Z_2$ -symmetric Ising model.

For values of  $\varphi$  for which the mass term  $m^2(\varphi) = \frac{1}{Z} \frac{\partial^2 U}{\partial \varphi^2}$  is much larger than  $\Lambda^2$  the microscopic approximation to  $\Gamma_k$  remains approximately valid also for  $k \rightarrow 0$ , i.e.  $U(\varphi) \approx U_\Lambda(\varphi)$ . The contribution of the long wavelength fluctuations is suppressed by the small correlation length or large mass. In the range where  $m^2(\varphi) \ll \Lambda^2$ , however, long distance fluctuations become important and perturbation theory loses its validity. Our aim is a description of this region by means of non-perturbative renormalization group techniques. Beyond the computation of universal critical exponents and amplitude ratios we want to establish an explicit connection between the universal critical equation of state and the microscopic free energy  $\Gamma_\Lambda$ .

In fig. 1 we plot our results for the equation of state near the endpoint of the critical line for carbon dioxide. For the microscopic scale we have chosen  $\Lambda^{-1} = 0.5 \text{ nm}$ . For  $\hat{\xi} = 0.6\Lambda^{-1}$ ,  $b_0(\Lambda) = 34 \text{ cm}^3 \text{ mol}^{-1}$ ,  $b_1(\Lambda) = 3.11 \cdot 10^6 \text{ bar cm}^6 \text{ mol}^{-2}$  we find the location of the endpoint at  $T_* = 307.4 \text{ K}$ ,  $p_* = 77.6 \text{ bar}$ ,  $\rho_* = 0.442 \text{ gcm}^{-3}$ . This compares well with the experimental values  $T_* = 304.15 \text{ K}$ ,  $p_* = 73.8 \text{ bar}$ ,  $\rho_* = 0.468 \text{ gcm}^{-3}$ . Comparing with literature values  $b_i(0)_{ld}$  for low density this yields  $b_0(\Lambda)/b_0(0)_{ld} = 0.8$ ,  $b_1(\Lambda)/b_1(0)_{ld} = 0.86$ . We conclude that the microscopic free energy can be approximated reasonably well by a van der Waals form even for high densities near  $n_*$ . The coefficients of the virial expansion are shifted compared to this low density values by 15-20 per cent. The comparison between the “microscopic equation of state” (dashed lines) and the true equation of state (solid lines) in the plot clearly demonstrates the importance of the fluctuations in the critical region. Away from the critical region the fluctuation effects are less significant and could be computed perturbatively.

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<sup>2</sup> Note that the source term is independent of  $k$ . The linear piece in the potential can therefore easily be added to  $U_{k \rightarrow 0}$  once all fluctuation effects are included.

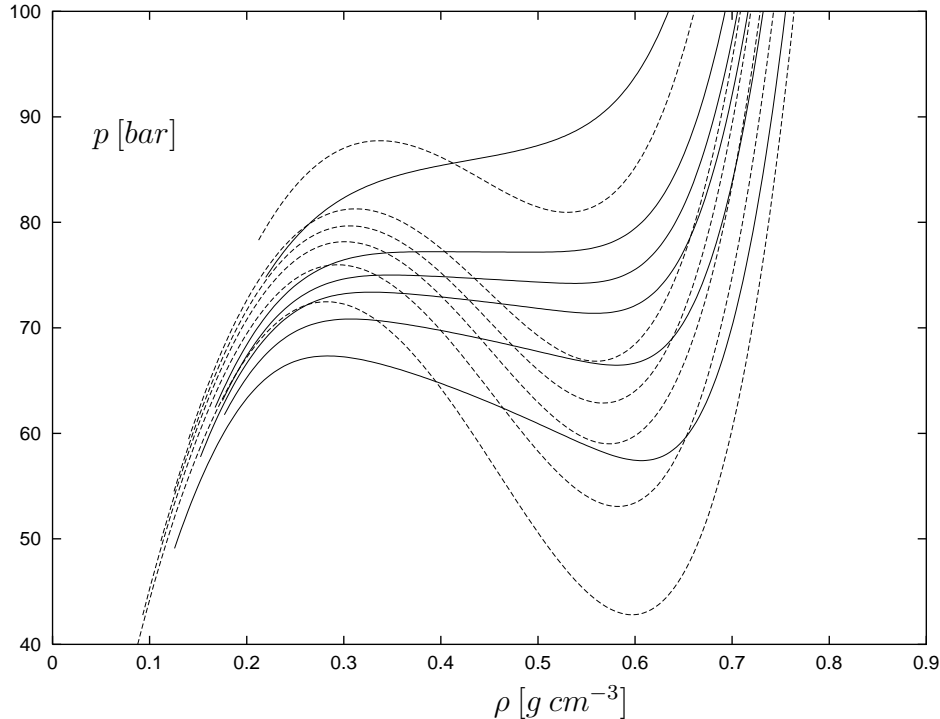


Figure 1:  $p$ – $\rho$ -isotherms of  $CO_2$  for  $T = 295K$ ,  $T = 300K$ ,  $T = 303K$ ,  $T = 305K$ ,  $T = 307K$  and  $T = 315K$ . The dashed lines represent the virial expansion (at the scale  $k = \Lambda$ ) in 2nd order with  $b_0 = 34 \text{ cm}^3 \text{ mol}^{-1}$ ,  $b_1 = 3.11 \cdot 10^6 \text{ bar cm}^6 \text{ mol}^{-2}$ . The solid lines are the results at the scale  $k = 0$  ( $\xi_\Lambda = 0.6$ ).

More details about the equation of state in the critical region as well as an explicit expression for  $U(n)$  will be presented in the following sections. In sect. 2 we briefly review our method and present the relevant non-perturbative flow equations. Sect. 3 is devoted to the critical behaviour of the Ising model. We compute the critical equation of state near the endpoint, critical indices, amplitudes and couplings. Our results compare well with sophisticated resummation methods of high order renormalization group improved perturbation theory, the  $\epsilon$ -expansion and high temperature series as well as with Monte-Carlo simulations and experiment. In this section we also give the universal behaviour of the  $\varphi$ -dependent wave function renormalization. This is needed for the dependence of the correlation length on density (or a magnetic field in magnets) and usually not available by other methods. In sect. 4 we turn to the equation of state for first order transitions. In the present case of the Ising universality class the universal features can be related to the second order phase transition in the Ising model. Such a simple connection is not available for more general systems.

Our flow equation can deal with first order transitions in an arbitrary context. We have computed here within a  $\varphi^4$ -model with cubic term and for the microscopic free energy (1.6). The perfect agreement with the Ising model predictions demonstrates the power of this method. The example of carbon dioxide shows the applicability for an arbitrary

form of the short-distance potential.

## 2 Flow equation for the effective potential

The dependence of the effective average action on the coarse graining scale  $k$  is described by an exact functional differential evolution equation [5]

$$\frac{\partial}{\partial k} \Gamma_k[\varphi] = \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \left\{ \left( \Gamma_k^{(2)}[\varphi] + R_k \right)^{-1} (q^2) \frac{\partial R_k(q^2)}{\partial k} \right\}. \quad (2.1)$$

It has the form of a renormalization group improved one-loop equation in ( $d$ -dimensional) momentum space. The diagonal elements of the effective average propagator, i.e.

$$\left( \Gamma_k^{(2)}[\varphi] + R_k \right)^{-1} (q', q) = \left( \Gamma_k^{(2)} + R_k \right)^{-1} (q^2) (2\pi)^d \delta(q' - q) + \text{off-diagonal terms},$$

involve the matrix of second functional derivatives of  $\Gamma_k$  with respect to the Fourier modes  $\varphi(q)$ , i.e.  $\delta^2 \Gamma_k[\varphi] / \delta \varphi(-q') \delta \varphi(q) = \Gamma_k^{(2)}[\varphi](q', q)$ .

For a suitable choice of  $R_k$  the momentum integral is both infrared and ultraviolet finite so that no additional regularization is needed and one can work in arbitrary dimension  $d$ . This flow equation is formally equivalent to other versions of exact renormalization group equations [3]. Using instead of the most general form of  $\Gamma$  the truncated ansatz (1.3) one extracts the (approximate) evolution equation for the potential by evaluating the flow equation for a constant field  $\varphi(q) = \varphi (2\pi)^d \delta(q)$ ,

$$\frac{\partial}{\partial t} U_k(\varphi) = v_d \int_0^\infty dx x^{\frac{d}{2}-1} \frac{\partial_t R_k(x)}{Z_k(\varphi)x + R_k(x) + \partial^2 U_k(\varphi) / \partial \varphi^2}. \quad (2.2)$$

Here  $t = \ln(k/\Lambda)$ ,  $x = q^2$ ,  $v_d^{-1} = 2^{d+1} \pi^{\frac{d}{2}} \Gamma(d/2)$ , and we choose a smooth infrared cutoff

$$R_k(x) = \frac{Z_{0,k} x}{\exp(x/k^2) - 1}. \quad (2.3)$$

The flow equation for  $Z_k(\varphi)$  can be obtained by adding to  $\varphi$  a small plane wave with long wavelength (see below). We note that the ansatz (1.3) can be regarded as the second order in a systematic derivative expansion for the solution of eq. (2.1). [7, 8]

Our aim is a numerical solution of the partial differential equation (2.2) with given initial conditions at the scale  $k \approx \Lambda$ . For this purpose it is convenient to introduce a dimensionless renormalized field

$$\tilde{\varphi} = k^{\frac{2-d}{2}} Z_{0,k}^{1/2} \varphi \quad (2.4)$$

with wave function renormalization  $Z_{0,k} = Z_k(\varphi_0(k))$  taken at the global potential minimum  $\varphi_0(k)$ . We also use

$$\begin{aligned} u_k(\tilde{\varphi}) &= k^{-d} U_k(\varphi) \\ \tilde{z}_k(\tilde{\varphi}) &= Z_{0,k}^{-1} Z_k(\varphi) \end{aligned} \quad (2.5)$$

and denote by  $u'$ ,  $\tilde{z}'$  the derivatives with respect to  $\tilde{\varphi}$ . This yields the scaling form of the flow equation for  $u'_k$ :

$$\begin{aligned} \frac{\partial}{\partial t} u'_k(\tilde{\varphi}) &= -\frac{1}{2}(d+2-\eta_0) \cdot u'_k(\tilde{\varphi}) + \frac{1}{2}(d-2+\eta_0) \tilde{\varphi} \cdot u''_k(\tilde{\varphi}) \\ &\quad - 2v_d \tilde{z}'_k(\tilde{\varphi}) \cdot l_1^{d+2}(u''_k(\tilde{\varphi}); \eta_0, \tilde{z}_k(\tilde{\varphi})) - 2v_d u'''_k(\tilde{\varphi}) \cdot l_1^d(u''_k(\tilde{\varphi}); \eta_0, \tilde{z}_k(\tilde{\varphi})). \end{aligned} \quad (2.6)$$

Similarly, the evolution of  $\tilde{z}_k$  is described in the truncation (1.3) by

$$\begin{aligned} \frac{\partial}{\partial t} \tilde{z}_k(\tilde{\varphi}) &= \eta_0 \cdot \tilde{z}_k(\tilde{\varphi}) + \frac{1}{2}(d-2+\eta_0) \tilde{\varphi} \cdot \tilde{z}'_k(\tilde{\varphi}) \\ &\quad - \frac{4}{d} v_d \cdot u'''_k(\tilde{\varphi})^2 \cdot m_{4,0}^d(u''_k(\tilde{\varphi}); \eta_0, \tilde{z}_k(\tilde{\varphi})) \\ &\quad - \frac{8}{d} v_d \cdot u'''_k(\tilde{\varphi}) \tilde{z}'_k(\tilde{\varphi}) \cdot m_{4,0}^{d+2}(u''_k(\tilde{\varphi}); \eta_0, \tilde{z}_k(\tilde{\varphi})) \\ &\quad - \frac{4}{d} v_d \cdot \tilde{z}'_k(\tilde{\varphi})^2 \cdot m_{4,0}^{d+4}(u''_k(\tilde{\varphi}); \eta_0, \tilde{z}_k(\tilde{\varphi})) - 2v_d \cdot \tilde{z}''_k(\tilde{\varphi}) \cdot l_1^d(u''_k(\tilde{\varphi}); \eta_0, \tilde{z}_k(\tilde{\varphi})) \\ &\quad + 4v_d \cdot \tilde{z}'_k(\tilde{\varphi}) u'''_k(\tilde{\varphi}) \cdot l_2^d(u''_k(\tilde{\varphi}); \eta_0, \tilde{z}_k(\tilde{\varphi})) \\ &\quad + \frac{2}{d}(1+2d)v_d \cdot \tilde{z}'_k(\tilde{\varphi})^2 \cdot l_2^{d+2}(u''_k(\tilde{\varphi}); \eta_0, \tilde{z}_k(\tilde{\varphi})) \end{aligned} \quad (2.7)$$

(see ref. [6] for the derivation of an analogous equation in a different language). Here the mass threshold functions

$$\begin{aligned} l_n^d(u''; \eta_0, \tilde{z}) &= -\frac{1}{2} k^{2n-d} \cdot Z_{0,k}^n \cdot \int_0^\infty dx x^{\frac{d}{2}-1} \tilde{\partial}_t \left\{ \frac{1}{(P(x) + Z_{0,k} k^2 u'')^n} \right\} \\ m_{n,0}^d(u''; \eta_0, \tilde{z}) &= -\frac{1}{2} k^{2(n-1)-d} \cdot Z_{0,k}^{n-2} \cdot \int_0^\infty dx x^{\frac{d}{2}} \tilde{\partial}_t \left\{ \frac{\dot{P}^2(x)}{(P(x) + Z_{0,k} k^2 u'')^n} \right\} \end{aligned} \quad (2.8)$$

(with  $P(x) = \tilde{z} Z_{0,k} x + R_k(x)$ ,  $\dot{P} \equiv \frac{dP}{dx}$  and  $\tilde{\partial}_t$  acting only on  $R_k$ ) describe the suppression of fluctuations once  $u''_k(\tilde{\varphi}) \gg 1$ . A discussion of their properties can be found in [7, 9]. The anomalous dimension

$$\eta_{0,k} \equiv -\frac{d}{dt} \ln Z_{0,k} = -Z_{0,k}^{-1} \frac{\partial}{\partial t} Z_k(\varphi_0) - Z_{0,k}^{-1} \cdot \frac{\partial Z_k}{\partial \varphi} \Big|_{\varphi_0} \cdot \frac{d\varphi_0}{dt} \quad (2.9)$$

is determined by the condition  $d\tilde{z}(\tilde{\varphi}_0)/dt = 0$ . It appears linearly in the threshold functions due to  $\tilde{\partial}_t$  acting on  $Z_{0,k}$  in the definition (2.3) of  $R_k$ .



For a computation of  $\eta_0$  we need the evolution of the potential minimum  $\varphi_0(k)$ , which follows from the condition  $\frac{d}{dt}(\partial U_k / \partial \varphi(\varphi_0(k))) = 0$ , namely

$$\begin{aligned} \frac{d\tilde{\varphi}_0}{dt} &= \frac{1}{2}(2 - d - \eta_0)\tilde{\varphi}_0 \\ &+ 2v_d \frac{\tilde{z}'_k(\tilde{\varphi}_0)}{u''_k(\tilde{\varphi}_0)} \cdot l_1^{d+2}(u''_k(\tilde{\varphi}_0); \eta_0, 1) + 2v_d \frac{u'''_k(\tilde{\varphi}_0)}{u''_k(\tilde{\varphi}_0)} \cdot l_1^d(u''_k(\tilde{\varphi}_0); \eta_0, 1). \end{aligned} \quad (2.10)$$

One infers an implicit equation for the anomalous dimension  $\eta_{0,k}$ ,

$$\begin{aligned} \eta_0 &= \frac{4}{d}v_d \cdot u'''_k(\tilde{\varphi}_0)^2 \cdot m_{4,0}^d(u''_k(\tilde{\varphi}_0); \eta_0, 1) + \frac{8}{d}v_d \cdot u'''_k(\tilde{\varphi}_0)\tilde{z}'_k(\tilde{\varphi}_0) \cdot m_{4,0}^{d+2}(u''_k(\tilde{\varphi}_0); \eta_0, 1) \\ &+ \frac{4}{d}v_d \cdot \tilde{z}'_k(\tilde{\varphi}_0)^2 \cdot m_{4,0}^{d+4}(u''_k(\tilde{\varphi}_0); \eta_0, 1) + 2v_d \cdot \tilde{z}''_k(\tilde{\varphi}_0) \cdot l_1^d(u''_k(\tilde{\varphi}_0); \eta_0, 1) \\ &- 4v_d \cdot \tilde{z}'_k(\tilde{\varphi}_0)u'''_k(\tilde{\varphi}_0) \cdot l_2^d(u''_k(\tilde{\varphi}_0); \eta_0, 1) \\ &- \frac{2}{d}(1 + 2d)v_d \cdot \tilde{z}'_k(\tilde{\varphi}_0)^2 \cdot l_2^{d+2}(u''_k(\tilde{\varphi}_0); \eta_0, 1) \\ &- 2v_d \frac{\tilde{z}'_k(\tilde{\varphi}_0)}{u''_k(\tilde{\varphi}_0)} \cdot \left\{ \tilde{z}'_k(\tilde{\varphi}_0)l_1^{d+2}(u''_k(\tilde{\varphi}_0); \eta_0, 1) + u'''_k(\tilde{\varphi}_0)l_1^d(u''_k(\tilde{\varphi}_0); \eta_0, 1) \right\}, \end{aligned} \quad (2.11)$$

that can be solved by separating the threshold functions in  $\eta_0$ -dependent and  $\eta_0$ -independent parts (c.f. eq. (2.8)). Since  $\eta_0$  will turn out to be only a few percent, the neglect of contributions from higher derivative terms not contained in (1.3) induces a substantial *relative* error for  $\eta_0$ , despite the good convergence of the derivative expansion. We believe that the missing higher derivative contributions to  $\eta_0$  constitute the main uncertainty in our results.

For given initial conditions  $U_\Lambda(\varphi)$ ,  $Z_\Lambda(\varphi)$  the system of partial differential equations (2.6),(2.7),(2.10),(2.11) can be solved numerically. A description of the algorithm used for the present work can be found in [9].

### 3 Critical equation of state for the Ising model

In order to make the discussion transparent we present here first results for polynomial initial conditions (1.10) with  $\tilde{z}_\Lambda(\tilde{\varphi}) = 1$ . The term linear in  $\varphi$  is considered as a source  $j$ . The special value  $\gamma_\Lambda = 0$  realizes the  $Z_2$ -symmetric Ising model. We start with the results for the universal critical behaviour for this case. For this particular purpose we hold  $\lambda_\Lambda$  fixed and measure the deviation from the critical temperature by

$$\delta m_\Lambda^2 = m_\Lambda^2 - m_{\Lambda,crit}^2 = S(T - T_c). \quad (3.1)$$

For the liquid-gas system one has  $S = 2b_1/(K_\Lambda^2 T_c^2)$ . As predicted by general scaling arguments we find that for small  $|\delta m_\Lambda^2|/\Lambda^2$  the susceptibility  $\chi = \bar{m}^{-1}$  and the inverse correlation length or renormalized mass  $m_R = \xi^{-1}$  in the high temperature phase ( $\delta m_\Lambda^2 > 0$ ) obey

$$\bar{m}^2 = (C^+)^{-1} \cdot (\delta m_\Lambda^2)^\gamma, \quad (3.2)$$

$$m_R = (\xi^+)^{-1} \cdot (\delta m_\Lambda^2)^\nu, \quad (3.3)$$

whereas for  $T < T_c$  one has

$$\bar{m}^2 = (C^-)^{-1} \cdot (-\delta m_\Lambda^2)^\gamma, \quad (3.4)$$

$$m_R = (\xi^-)^{-1} \cdot (-\delta m_\Lambda^2)^\nu. \quad (3.5)$$

Here the renormalized and unrenormalized squared mass terms are defined by

$$\bar{m}^2 = \frac{\partial^2 U}{\partial \varphi^2}(\varphi_0), \quad m_R^2 = \frac{\partial^2 U}{\partial \varphi_R^2}(\varphi_0), \quad \varphi_R = Z_0^{1/2} \varphi. \quad (3.6)$$

While for  $T > T_c$  the minimum of  $U = U_{k \rightarrow 0}$  is at the symmetric point  $\varphi_0 = 0$ , the low temperature phase is characterized by spontaneous symmetry breaking, with

$$\varphi_0 = B \cdot (-\delta m_\Lambda^2)^\beta, \quad (3.7)$$

$$\varphi_{0R}^2 = 2E \cdot (-\delta m_\Lambda^2)^\nu. \quad (3.8)$$

The anomalous dimension  $\eta$  determines the two point function at the critical temperature and equals  $\eta_{0,k}$  for the scaling solution where  $\partial_t u = \partial_t \tilde{z} = 0$ . Our results for the critical exponents are compared with those from other methods in table 3. We observe a very good agreement for  $\nu$  whereas the relative error for  $\eta$  is comparatively large as expected. Comparison with the lowest order of the derivative expansion (f) shows a convincing apparent convergence of this expansion for  $\nu$ . For  $\eta$  this convergence is hidden by the fact that in [10] a different determination of  $\eta$  was used. Employing the present definition would lead in lowest order of the derivative expansion to a value  $\eta = 0.11$ . As expected, the convergence of the derivative expansion is faster for the very effective exponential cutoff than for the powerlike cutoff (g) which would lead to unwanted properties of the momentum integrals in the next order.

In order to establish the quantitative connection between the short distance parameters  $m_\Lambda^2$  and  $\lambda_\Lambda$  and the universal critical behaviour one needs the amplitudes  $C^\pm$ ,  $\xi^\pm$ , etc. For  $\lambda_\Lambda/\Lambda = 5$  we find  $C^+ = 1.033$ ,  $C^- = 0.208$ ,  $\xi^+ = 0.981$ ,  $\xi^- = 0.484$ ,  $B = 0.608$ ,  $E = 0.208$ . Here and in the following all dimensionful quantities are quoted in units of  $\Lambda$ . The amplitude  $D$  is given by  $\partial U_0/\partial \varphi = D \cdot \varphi^\delta$  on the critical isotherme and we obtain  $D = 10.213$ . In table 2 we present our results for the universal amplitude ratios  $C^+/C^-$ ,  $\xi^+/\xi^-$ ,  $R_\chi = C^+ D B^{\delta-1}$ ,  $\tilde{R}_\xi = (\xi^+)^{\beta/\nu} D^{1/(\delta+1)} B$ .

The critical exponents and amplitudes only characterize the behaviour of  $U(\varphi)$  in the limits  $\varphi \rightarrow \varphi_0$  and  $\varphi \rightarrow \infty$ . Our method allows us to compute  $U(\varphi)$  for arbitrary  $\varphi$ . As an example, the quartic coupling  $\lambda_R = \frac{1}{3} \frac{\partial^4 U}{\partial \varphi_R^4}(0) = \frac{\partial^2 U}{\partial \rho_R^2}(0)$ ,  $\hat{\lambda}_R = \frac{\partial^2 U}{\partial \rho_R^2}(\varphi_{0R})$ ,  $\rho_R = \frac{1}{2} \varphi_R^2$ ,

	$\nu$	$\beta$	$\gamma$	$\eta$
(a)	0.6304(13)	0.3258(14)	1.2397(13)	0.0335(25)
(b)	0.6293(26)	0.3260(20)	1.2360(40)	0.036(6)
(c)	0.6300(49)		1.2400(87)	
(d)	0.625(1)			0.025(6)
(e)	0.629(3)			0.027(5)
(f)	0.643	0.336	1.258	0.044
(g)	0.6181			0.054
(h)	0.6307	0.3300	1.2322	0.0467
(i)	0.625(6)	0.316 – 0.327	1.23 – 1.25	

Table 1: Critical exponents of the ( $d=3$ )-Ising model, calculated with various methods.

(a) Six loop resummed perturbation series at fixed dimension  $d = 3$  [4, 14].

(b)  $\epsilon$ -expansion in five loop order [4, 14], (c) high temperature series [15] (see also [16], [17]).

(d),(e) Monte Carlo simulations [18]- [20].

(f)-(h): “exact” renormalization group equations.

(f) effective average action for the  $O(N)$ -model,  $N \rightarrow 1$ , with uniform wave function renormalization [10] (see also [7]).

(g) scaling solution of equations analogous to (2.6), (2.7) with powerlike cutoff [8].

(h) effective average action for one-component scalar field theory with field-dependent wave function renormalization (present work).

(i) experimental data for the liquid-vapour system quoted from [4]

becomes in the critical region proportional to  $m_R$ . Our results for the universal couplings  $\lambda_R/m_R$  in the symmetric and  $\hat{\lambda}_R/\hat{m}_R$  in the ordered phase can also be found in table 2. Here  $m_R = \frac{\partial^2 U}{\partial \varphi_R^2} \big|_{\varphi_R=0}$  in the symmetric and  $\hat{m}_R = \frac{\partial^2 U}{\partial \varphi_R^2} \big|_{\varphi_{0R}}$  in the ordered phase.

We should emphasize that the shape of the potential in the low temperature phase depends on  $k$  in the “inner” region corresponding to  $|\varphi| < \varphi_0$ . This is due to the fluctuations which are responsible for making the potential convex in the limit  $k \rightarrow 0$  [11, 12, 13]. We illustrate this by plotting the potential for different values of  $k$  in fig. 2.

In the universal critical region the expectation value of  $\varphi$  for very small  $|\delta m_\Lambda^2|$  and sources  $j$  (with  $\partial U/\partial \varphi(\varphi_j) = j$ ) can be found from the Widom scaling form of the equation of state

$$\frac{\partial}{\partial \varphi} U(\varphi) = |\varphi|^\delta f(x) \cdot \Lambda^{\frac{5-\delta}{2}} \quad (3.9)$$

$$x = \frac{\delta m_\Lambda^2}{|\varphi|^{1/\beta}} \cdot \Lambda^{\frac{1}{2\beta}-2}. \quad (3.10)$$

Our results for the scaling function  $f(x)$  are shown in fig. 3, together with the asymptotic behaviour (dashed lines) as dictated by the critical exponents and amplitudes:

$$\begin{aligned} \lim_{x \rightarrow 0} f(x) = D \quad , \quad f(x = -B^{-1/\beta}) = 0, \\ \lim_{x \rightarrow \infty} f(x) = (C^+)^{-1} x^\gamma \quad , \quad \lim_{x \rightarrow -\infty} f(x) = (C^-)^{-1} (-x)^\gamma \end{aligned} \quad (3.11)$$

	$C^+/C^-$	$\xi^+/\xi^-$	$R_\chi$	$\tilde{R}_\xi$	$\xi^+E$	$\lambda_R/m_R$	$\hat{\lambda}_R/\hat{m}_R$
(a)	$4.79 \pm 0.10$		$1.669 \pm 0.018$			7.88	
(b)	$4.72 \pm 0.14$		$1.648 \pm 0.031$			9.33	
(c)	$4.95 \pm 0.015$	$1.96 \pm 0.01$	1.75			$7.9 - 8.15$	
(d)	$4.75 \pm 0.03$	$1.95 \pm 0.02$				7.76	5.27
(f)	4.29	1.86	1.61	0.865	0.168	9.69	5.55
(h)	4.966	2.027	1.647	0.903	0.204	8.11	4.96
(i)	$4.8 - 5.2$		$1.69 \pm 0.14$				

Table 2: Universal amplitude ratios and couplings of the ( $d=3$ )-Ising model.

- (a) perturbation theory at fixed dimension  $d=3$  [14], (b)  $\epsilon$ -expansion [14].  
(c) high temperature series. Amplitude ratios from [4],  $\lambda_R/m_R$  from [15, 16, 17].  
(d) Monte Carlo simulations. Amplitude ratios from [20],  $\hat{\lambda}_R/\hat{m}_R$  from [19],  $\lambda_R/m_R$  from [18].  
(f) effective average action for the  $O(N)$ -model,  $N \rightarrow 1$ , with uniform wave function renormalization [10].  
(h) present work with field-dependent wave function renormalization.  
(i) experimental data for the liquid-vapour system [21].

where

$$(C^-)^{-1} = B^{\delta-1-1/\beta} \frac{1}{\beta} f'(-B^{-1/\beta}) \quad , \quad f'(x) = \frac{\beta}{x} \cdot \left( \delta f(x) - \frac{\partial^2 U}{\partial \varphi^2} \varphi^{1-\delta} \right). \quad (3.12)$$

We have verified the scaling form of the equation of state explicitly by starting with a large variety of initial conditions (e.g. different  $\lambda_\Lambda$ ).

A different useful parameterization of the critical equation of state can be given in terms of nonlinearly rescaled fields  $\hat{\varphi}_R$ , using a  $\varphi$ -dependent wave function renormalization  $Z(\varphi) = Z_{k \rightarrow 0}(\varphi)$ ,

$$\hat{\varphi}_R = Z(\varphi)^{1/2} \varphi. \quad (3.13)$$

Our numerical results can be presented in terms of a fit to the universal function

$$\hat{F}(\hat{s}) = m_R^{-5/2} \frac{\partial U}{\partial \hat{\varphi}_R} \quad , \quad \hat{s} = \frac{\hat{\varphi}_R}{m_R^{1/2}} = \left( \frac{Z(\varphi) \varphi^2}{m_R} \right)^{1/2}, \quad (3.14)$$

$$\hat{F}_{Fit}(\hat{s}) = (a_0 \hat{s} + a_1 \hat{s}^3 + a_2 \hat{s}^5 + a_3 \hat{s}^7) \cdot f_\alpha(\hat{s}) + (1 - f_\alpha(\hat{s})) \cdot a_4 \hat{s}^5. \quad (3.15)$$

The factors  $f_\alpha$  and  $(1-f_\alpha)$  interpolate between a polynomial expansion and the asymptotic behaviour for large arguments. We use

$$f_\alpha(x) = \alpha^{-2} x^2 \cdot \frac{\exp(-\frac{x^2}{\alpha^2})}{1 - \exp(-\frac{x^2}{\alpha^2})}. \quad (3.16)$$

A similar fit can be given for

$$\tilde{z}(s) = \frac{\lim_{k \rightarrow 0} Z_k(\varphi)}{Z_0} \quad , \quad s = \frac{\varphi_R}{m_R^{1/2}} = \left( \frac{Z_0 \varphi^2}{m_R} \right)^{1/2} = \tilde{z}^{-1/2} \hat{s}, \quad (3.17)$$

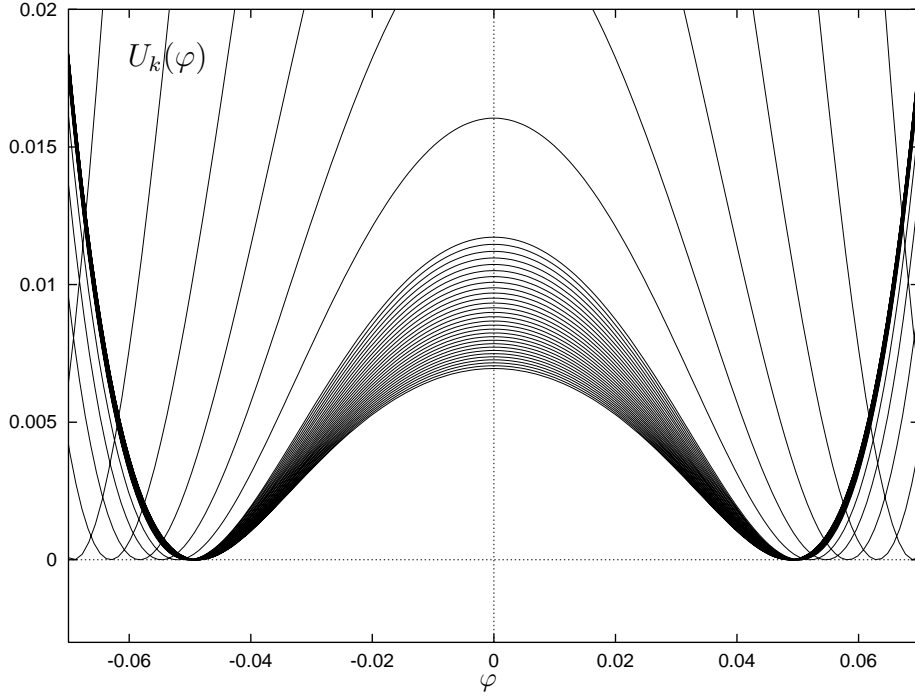


Figure 2:  $U_k(\varphi)$  for different scales  $k$ . The shape of  $U$  is stored in smaller intervals  $\Delta t = -0.02$  after leaving the scaling solution. This demonstrates the approach to convexity in the “inner region”, while the “outer region” becomes  $k$ -independent.

$$\tilde{z}_{Fit}(s) = (b_0 + b_1 s^2 + b_2 s^4 + b_3 s^6 + b_4 s^8) \cdot f_\beta(s) + (1 - f_\beta(s)) \cdot b_5 |s|^{-\frac{2\eta}{1+\eta}}. \quad (3.18)$$

In the symmetric phase one finds (with  $\eta = 0.0467$ )  $\alpha = 1.012$ ,  $a_0 = 1.0084$ ,  $a_1 = 3.1927$ ,  $a_2 = 9.7076$ ,  $a_3 = 0.5196$ ,  $a_4 = 10.3962$  and  $\beta = 0.5103$ ,  $b_0 = 1$ ,  $b_1 = 0.3397$ ,  $b_2 = -0.8851$ ,  $b_3 = 0.8097$ ,  $b_4 = -0.2728$ ,  $b_5 = 1.0717$ , whereas the fit parameters for the phase with spontaneous symmetry breaking are  $\alpha = 0.709$ ,  $a_0 = -0.0707$ ,  $a_1 = -2.4603$ ,  $a_2 = 11.8447$ ,  $a_3 = -1.3757$ ,  $a_4 = 10.2115$  and  $\beta = 0.486$ ,  $b_0 = 1.2480$ ,  $b_1 = -1.4303$ ,  $b_2 = 2.3865$ ,  $b_3 = -1.7726$ ,  $b_4 = 0.4904$ ,  $b_5 = 0.8676$  (our fit parameters are evaluated for this phase for  $(\partial^2 U / \partial \varphi_R^2)(\varphi_{R,max}) / k^2 = -0.99$ ). One observes that the coefficients  $a_2$  and  $a_4$  are large and of comparable size. A simple polynomial form  $\hat{F} = \tilde{a}_0 \hat{s} + \tilde{a}_1 \hat{s}^3 + \tilde{a}_2 \hat{s}^5$  is not too far from the more precise result. We conclude that in terms of the rescaled field  $\hat{\varphi}_R$  (3.13) the potential is almost a polynomial  $\varphi^6$ -potential.

In fig. 4 we show  $\tilde{z}$  as a function of  $s$  both for the symmetric and ordered phase. Their shape is similar to the scaling solution found in [8]. Nevertheless, the form of  $\tilde{z}$  for  $k = 0$  which expresses directly information about the physical system should not be confounded with the scaling solution which depends on the particular infrared cutoff. For the low temperature phase one sees the substantial dependence of  $\tilde{z}_k$  on the infrared cutoff  $k$  for small values  $s < s_0$ . Again this corresponds to the “inner region” between the origin ( $s=0$ ) and the minimum of the potential ( $s_0=0.449$ ) where the potential finally becomes

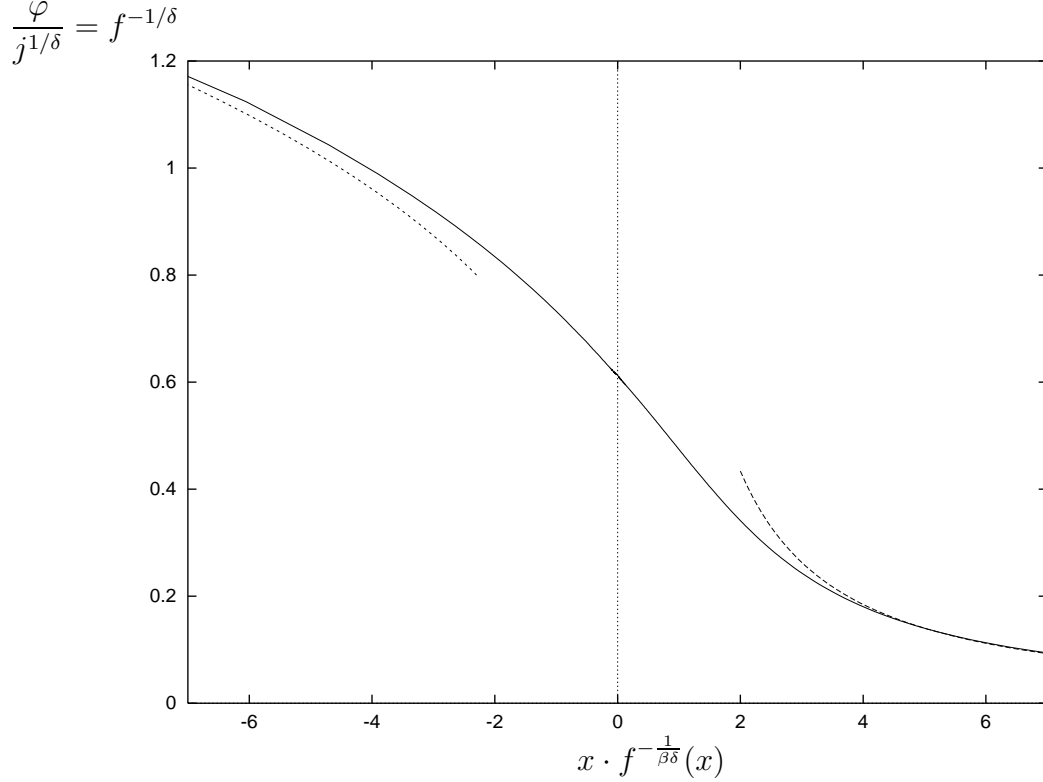


Figure 3: Widom scaling function  $f(x)$  of the  $(d=3)$ -Ising model. ( The present curve is generated for a quartic short distance potential  $U_\Lambda$  with  $\lambda_\Lambda/\Lambda = 5$ ). The dashed lines indicate extrapolations of the limiting behaviour as given by the critical exponents.

convex for  $k \rightarrow 0$ .

Knowledge of  $U$  and  $\tilde{z}$  permits the computation of the (renormalized) propagator for low momenta with arbitrary sources  $j$ . It is given by

$$G(q^2) = \left( \frac{\partial^2 U(\varphi_R)}{\partial \varphi_R^2} + \tilde{z}(\varphi_R) q^2 \right)^{-1} \quad (3.19)$$

for  $\tilde{z} q^2 \lesssim \partial^2 U / \partial \varphi_R^2$ . Here  $\varphi_R$  obeys  $\partial U / \partial \varphi_R = Z_0^{-1/2} j$ . We emphasize that the correlation length  $\xi(\varphi_R) = \tilde{z}^{1/2}(\varphi_R) (\partial^2 U / \partial \varphi_R^2)^{-1/2}$  at given source  $j$  requires information about  $\tilde{z}$ . For the gas-liquid transition  $\xi(\varphi_R)$  is directly connected to the density dependence of the correlation length. For magnets, it expresses the correlation length as a function of magnetization. The factor  $\tilde{z}^{1/2}$  is often omitted in other approaches.

Critical equations of state for the Ising model have been computed earlier with several methods. They are compared with our result for the phase with spontaneous symmetry breaking in fig. 5 and for the symmetric phase in fig. 6. For this purpose we use  $F(\tilde{s}) = m_R^{-5/2} \partial U / \partial \varphi_R$  with  $\tilde{s} = \frac{\varphi_R}{\varphi_{0R}}$  in the phase with spontaneous symmetry breaking (note  $\tilde{s} \sim s$ ). The constant  $c_F$  is adapted such that  $\frac{1}{c_F} \frac{\partial F}{\partial \tilde{s}}(\tilde{s}=1) = 1$ . In the symmetric phase we take instead  $\tilde{s} = \frac{\varphi_R}{m_R^{5/2}}$  such that  $\frac{\partial F}{\partial \tilde{s}}(\tilde{s}=0) = 1$ . One expects for large  $\tilde{s}$  an inaccuracy of our results due to the error in  $\eta$ .

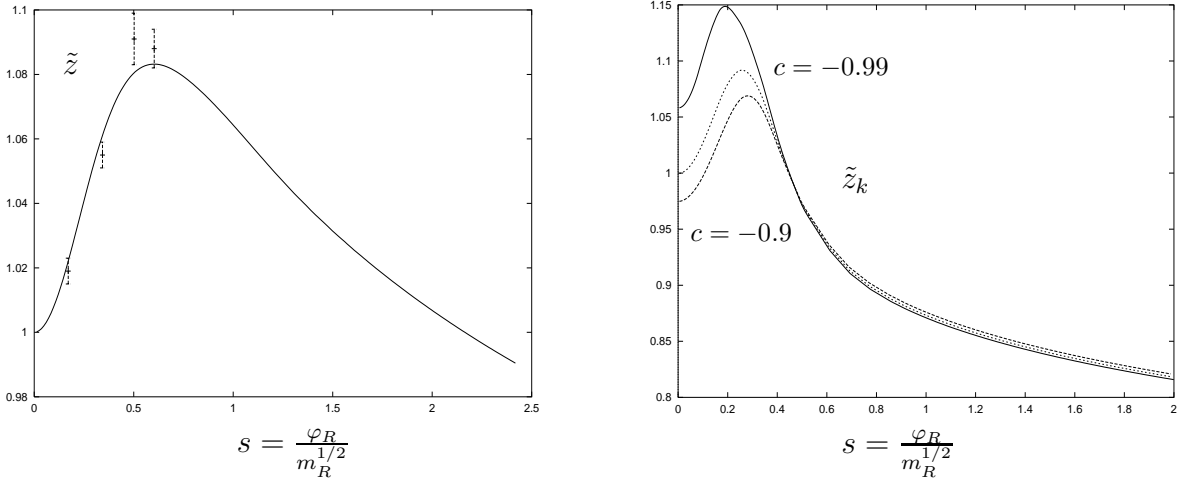


Figure 4: Universal rescaled wave function renormalization  $\tilde{z}$  in the symmetric and ordered phase of the  $(d=3)$ -Ising model. In the low temperature phase the plots are for different  $k$  with  $\frac{1}{k^2} \frac{\partial^2 U}{\partial \varphi_R^2}(\varphi_{R,max}) = c$  ( $c = -0.9, -0.95, -0.99$ ). Here  $\varphi_{R,max}$  is the location of the local maximum of the potential in the inner (non-convex) region. In the graph for the high temperature phase we have inserted Monte Carlo results by M. Tsy-pin (private communication).

	$m_{\Lambda,crit}^2$	$C^+$	D
$\lambda_\Lambda = 0.1$	$-6.4584 \cdot 10^{-3}$	0.1655	5.3317
$\lambda_\Lambda = 1$	$-5.5945 \cdot 10^{-2}$	0.485	7.506
$\lambda_\Lambda = 5$	-0.22134	1.033	10.213
$\lambda_\Lambda = 20$	-0.63875	1.848	16.327

Table 3: The critical values  $m_{\Lambda,crit}^2$  and the non-universal amplitudes  $C^+$ ,  $D$  as a function of the quartic short distance coupling  $\lambda_\Lambda$  (all values expressed in units of  $\Lambda$ ). Other non-universal amplitudes can be calculated from the universal quantities of table 2.

In summary of this section we may state that the non-perturbative flow equations in second order in a derivative expansion lead to a critical equation of state which is well compatible with high order expansions within other methods. In addition, it allows to establish an explicit connection between the parameters appearing in the microscopic free energy  $\Gamma_\Lambda$  and the universal long distance behaviour. For a quartic polynomial potential this involves in addition to the non-universal amplitudes the value of  $m_{\Lambda,crit}^2$ . We have listed these quantities for different values of  $\lambda_\Lambda$  in table 3. Finally, the temperature scale is established by  $S = \partial m_\Lambda^2 / \partial T |_{T_c}$ .

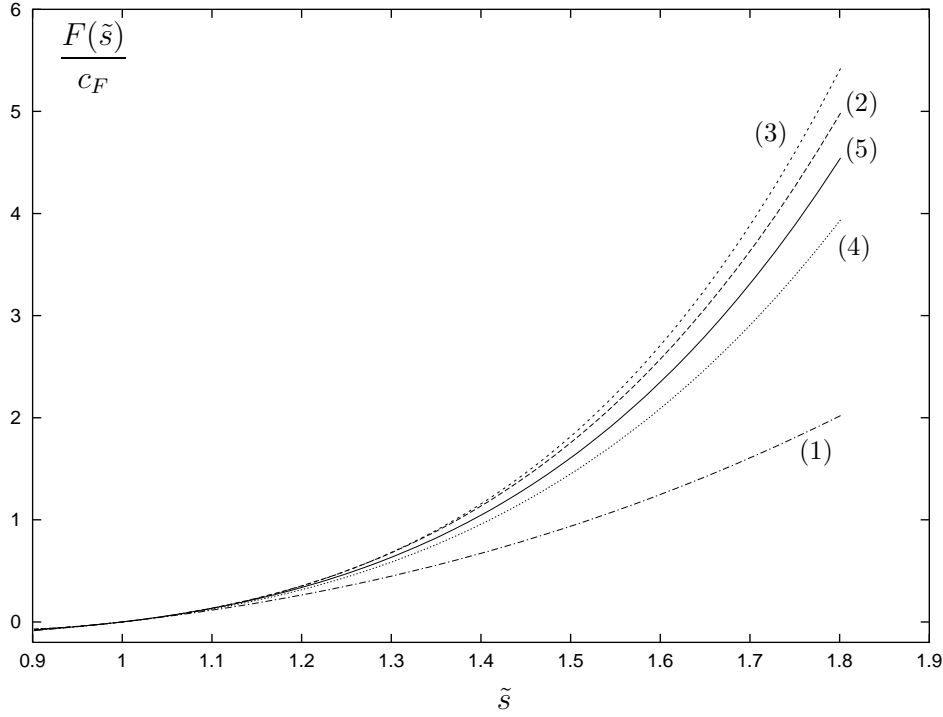


Figure 5: The critical equation of state in the ordered phase.

- (1) mean field approximation.
- (2) effective average action with uniform wave function renormalization [10].
- (3) Monte Carlo simulation [19].
- (4) resummed  $\epsilon$ -expansion in  $O(\epsilon^3)$ , five loop perturbative expansion and high temperature series [14].
- (5) present work.

## 4 Equation of state for first order transitions

Our method is not restricted to a microscopic potential with discrete  $Z_2$ -symmetry. The numerical code works for arbitrary initial potentials. We have investigated the polynomial potential (1.10) with  $\gamma_\Lambda \neq 0$ . The numerical solution of the flow equations (2.6),(2.7) shows the expected first order transition (in case of vanishing linear term  $j$ ). Quite generally, the universal critical equation of state for first order transitions will depend on two scaling parameters (instead of one for second order transitions) since the jump in the order parameter or the mass introduces a new scale. The degree to which universality applies depends on the properties of a given model and its parameters (see [9, 10] for a detailed discussion). For a  $\varphi^4$ -model with cubic term (1.10) one can relate the equation of state to the Ising model by an appropriate mapping. This allows us to compute the universal critical equation of state for arbitrary first order phase transitions in the Ising universality class from the critical equation of state for the second order phase transition in the Ising model. For other universality classes a simple mapping to a second order equation of state is not always possible - its existence is particular to the present model.



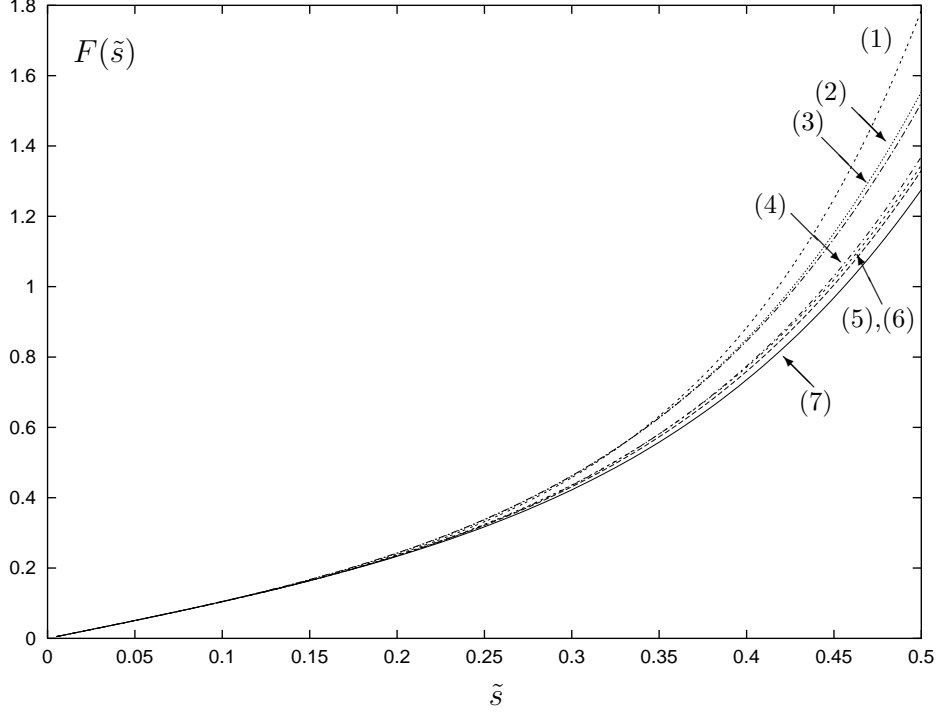


Figure 6: The critical equation of state in the symmetric phase.

- (1) Monte Carlo simulation [22], (2)  $\epsilon$ -expansion [14].  
(3) effective average action with uniform wave function renormalization [10].  
(4) Monte Carlo simulation [18], (5),(6) high temperature series [17],[16].  
(7) present work.

By a variable shift

$$\sigma = \varphi + \frac{\gamma_\Lambda}{3\lambda_\Lambda} \quad (4.1)$$

we can bring the short distance potential (1.10) into the form

$$U_\Lambda(\sigma) = -J_\gamma \sigma + \frac{\mu_\Lambda^2}{2} \sigma^2 + \frac{\lambda_\Lambda}{8} \sigma^4 + c_\Lambda \quad (4.2)$$

with

$$\begin{aligned} J_\gamma &= \frac{\gamma_\Lambda}{3\lambda_\Lambda} m_\Lambda^2 - \frac{\gamma_\Lambda^3}{27\lambda_\Lambda^2} \\ \mu_\Lambda^2 &= m_\Lambda^2 - \frac{\gamma_\Lambda^2}{6\lambda_\Lambda}. \end{aligned} \quad (4.3)$$

We can now solve the flow equations in terms of  $\sigma$  and reexpress the result in terms of  $\varphi$  by eq. (4.1) at the end. The exact flow equation (2.1) does not involve the linear term  $\sim J_\gamma \sigma$  on the right hand side (also the constant  $c_\Lambda$  is irrelevant). Therefore the effective potential ( $k=0$ ) is given by

$$U = U^{Z_2}(\sigma) - J_\gamma \sigma + c_\Lambda = U^{Z_2}(\varphi + \frac{\gamma_\Lambda}{3\lambda_\Lambda}) - (\varphi + \frac{\gamma_\Lambda}{3\lambda_\Lambda}) J_\gamma + c_\Lambda, \quad (4.4)$$

where  $U^{Z_2}$  is the effective potential of the Ising type model with quartic coupling  $\lambda_\Lambda$  and mass term  $\mu_\Lambda^2$ . The equation of state  $\partial U/\partial\varphi = j$  or, equivalently

$$\frac{\partial U^{Z_2}}{\partial\varphi} \Big|_{\varphi+\frac{\gamma_\Lambda}{3\lambda_\Lambda}} = j + J_\gamma, \quad (4.5)$$

is therefore known explicitly for arbitrary  $m_\Lambda^2$ ,  $\gamma_\Lambda$  and  $\lambda_\Lambda$  (cf. eq. (3.9) for the universal part). This leads immediately to the following conclusions:

- i) First order transitions require that the combination  $U(\varphi) - j\varphi$  has two degenerate minima. This happens for  $J_\gamma + j = 0$  and  $\mu_\Lambda^2 < \mu_{\Lambda,crit}^2$  or

$$j = -\frac{\gamma_\Lambda}{3\lambda_\Lambda} \left( m_\Lambda^2 - \frac{\gamma_\Lambda^2}{9\lambda_\Lambda} \right) \quad (4.6)$$

$$m_\Lambda^2 < \mu_{\Lambda,crit}^2 + \frac{\gamma_\Lambda^2}{6\lambda_\Lambda}. \quad (4.7)$$

Here  $\mu_{\Lambda,crit}^2$  is the critical mass term of the Ising model.

- ii) The boundary of this region for

$$m_\Lambda^2 = \mu_{\Lambda,crit}^2 + \frac{\gamma_\Lambda^2}{6\lambda_\Lambda} \quad (4.8)$$

is a line of second order phase transitions with vanishing renormalized mass or infinite correlation length.

For  $j = 0$  (e.g. magnets with polynomial potential in absence of external fields) the equations (4.6), (4.8) have the solutions

$$\gamma_{\Lambda;1} = 0 \quad , \quad \gamma_{\Lambda;2,3} = \pm(-18\lambda_\Lambda\mu_{\Lambda,crit}^2)^{1/2}. \quad (4.9)$$

The second order phase transition for  $\gamma_\Lambda \neq 0$  can be described by Ising models for shifted fields  $\sigma$ . For a given model, the way how a phase transition line is crossed as the temperature is varied follows from the temperature dependence of  $j$ ,  $m_\Lambda^2$ ,  $\gamma_\Lambda$  and  $\lambda_\Lambda$ . For the gas-liquid transition both  $j$  and  $m_\Lambda^2$  depend on  $T$ .

In the vicinity of the boundary of the region of first order transitions the long range fluctuations play a dominant role and one expects universal critical behaviour. The detailed microscopic physics is only reflected in two non-universal amplitudes. One reflects the relation between the renormalized and unrenormalized fields as given by  $Z_0$ . The other is connected to the renormalization factor for the mass term. Expressed in terms of renormalized fields and mass the potential  $U$  loses all memory about the microphysics.

The critical equation of state of the non-symmetric model ( $\gamma_\Lambda \neq 0$ ) follows from the Ising model (4.5). With  $\frac{\partial U^{Z_2}}{\partial\varphi} \Big|_\varphi = |\varphi|^\delta f(x)$ , the scaling form of the equation of state  $j = \frac{\partial U}{\partial\varphi}$  for the model with cubic coupling can be written as

$$j = |\varphi + \frac{\gamma_\Lambda}{3\lambda_\Lambda}|^\delta f(x) - \left( \frac{\gamma_\Lambda}{3\lambda_\Lambda} \mu_{\Lambda,crit}^2 + \frac{\gamma_\Lambda^3}{54\lambda_\Lambda^2} \right) - \frac{\gamma_\Lambda}{3\lambda_\Lambda} \delta \mu_\Lambda^2, \quad (4.10)$$

where  $x = \frac{\delta\mu_\Lambda^2}{|\varphi + \frac{\gamma_\Lambda}{3\lambda_\Lambda}|^{1/\beta}}$  and  $\delta\mu_\Lambda^2 = m_\Lambda^2 - \frac{\gamma_\Lambda^2}{6\lambda_\Lambda} - \mu_{\Lambda,crit}^2$ . One may choose

$$y = \frac{\gamma_\Lambda}{3\lambda_\Lambda} \left( \mu_{\Lambda,crit}^2 + \frac{\gamma_\Lambda^2}{18\lambda_\Lambda} + \delta\mu_\Lambda^2 \right) |\varphi + \frac{\gamma_\Lambda}{3\lambda_\Lambda}|^{-\delta} \quad (4.11)$$

as the second scaling variable. For small symmetry breaking cubic coupling  $\gamma_\Lambda$  one notes  $y \sim \gamma_\Lambda$ . The scaling form of the equation of state for the non-symmetric model reads

$$j = |\varphi + \frac{\gamma_\Lambda}{3\lambda_\Lambda}|^\delta \{f(x) - y\}. \quad (4.12)$$

This universal form of the equation of state is relevant for a large class of microscopic free energies, far beyond the special polynomial form used for its derivation.

It is often useful to express the universal equation of state in terms of renormalized fields and masses. We use the variables

$$\tilde{s} = \frac{\varphi_R}{\varphi_{0R}} \quad ; \quad v = \frac{m_R}{m_R^{Z_2}}, \quad (4.13)$$

where  $m_R = \left( \frac{\partial^2 U}{\partial \varphi_R^2} \big|_{\varphi_{0R}} \right)^{1/2}$  is the renormalized mass at the minimum  $\varphi_{0R}$  of  $U(\varphi_R)$  whereas  $m_R^{Z_2}$  is the renormalized mass at the minimum of the corresponding  $Z_2$ -symmetric effective potential obtained for vanishing cubic coupling  $\gamma_\Lambda = 0$ . Then the critical temperature corresponds to  $v = 1$ . In this parameterization the universal properties of the equation of state for the Ising type first order transition can be compared with transitions in other models - e.g. matrix models [9] - where no simple mapping to a second order phase transition exists.

A convenient universal function  $G(\tilde{s}, v)$  for weak first order transitions can be defined as

$$G(\tilde{s}, v) := \frac{U(\varphi_R)}{\varphi_{0R}^6}. \quad (4.14)$$

We plot  $G(\tilde{s}, v)$  in fig. 7 as a function of  $\tilde{s}$  for different values of  $v$ . For the present model all information necessary for a universal description of first order phase transitions is already contained in eqs. (4.4) or (4.5). The function  $G(\tilde{s}, v)$  can serve, however, for a comparison with other models. At this place we mention that we have actually computed the potential  $U$  both by solving the flow equations with initial values where  $\gamma_\Lambda \neq 0$  and by a shift from the Ising model results. We found good agreement between the two approaches.

## 5 Discussion

In conclusion, we have employed non-perturbative flow equations in order to compute explicitly the equation of state. We have first studied models where the microscopic free energy can be approximated by a polynomial approximation with terms up to quartic

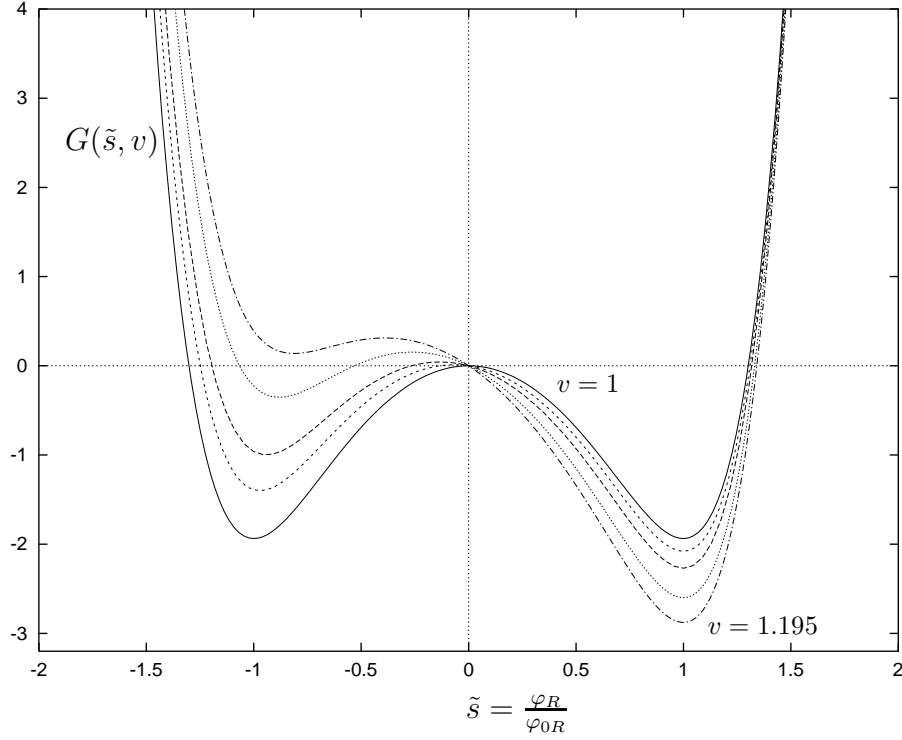


Figure 7:  $G(\tilde{s}, v)$  for  $v = 1$ ,  $v = 1.037$ ,  $v = 1.072$ ,  $v = 1.137$  and  $v = 1.195$ .

order. This covers second order as well as first order transitions, both for the universal and non-universal features. The same method can be used away from the critical hypersurface, allowing therefore for an explicit connection between critical and non-critical observations.

The ability of the method to deal also with a microscopic free energy which is not of a polynomial form is demonstrated by a particular example, namely the equation of state for carbon dioxide. In the vicinity of the endpoint of the critical line we can give an explicit formula for the free energy density  $U(n, T)T$ . Using the fits (3.15), ((3.18), for  $\hat{F}(\hat{s})$  and  $\tilde{z}(s)$  one finds<sup>3</sup>

$$U(n, T) = U^{Z_2}(\hat{\varphi}_R(n, T), m_R(T)) + J(T)(n - n_*) - K(T) \quad (5.1)$$

$$U^{Z_2} = \frac{1}{2}\tilde{a}_0 m_R^2 \hat{\varphi}_R^2 + \frac{1}{4}\tilde{a}_1 m_R \hat{\varphi}_R^4 + \frac{1}{6}\tilde{a}_2 \hat{\varphi}_R^6 \quad (5.2)$$

with  $\tilde{a}_i \approx a_i$  and

$$\hat{\varphi}_R(n, T) = \tilde{z}\left(\frac{\varphi_R(n, T)}{m_R^{1/2}(T)}\right) \varphi_R(n, T)$$

---

<sup>3</sup>Note that  $n_*$  is somewhat different from  $\hat{n}$  and therefore  $\varphi_R$  is defined slightly different from eq. (1.7). This variable shift (similar to (4.1) reflects the fact that eq. (1.6) contains higher than quartic interactions and cannot be reduced to a  $\varphi^4$ -potential even for  $\gamma_\Lambda = 0$ .

$$\begin{aligned}
\varphi_R(n, T) &= H_{\pm} \left| \frac{T - T_*}{T_*} \right|^{-\eta\nu} (n - n_*) \\
m_R(T) &= \xi_{T\pm} \left| \frac{T - T_*}{T_*} \right|^{\nu}
\end{aligned} \tag{5.3}$$

The two non-universal functions  $J(T)$  and  $K(T)$  enter in the determination of the chemical potential and the critical line.

In particular, the nonuniversal amplitudes governing the behaviour near the endpoint of the critical line can be extracted from the equation of state: In the vicinity of the endpoint we find for  $T = T_*$

$$\rho_{>} - \rho_* = \rho_* - \rho_{<} = D_p^{-1} \left( \frac{|p - p_*|}{p_*} \right)^{1/\delta} \tag{5.4}$$

with  $D_p = 2.8 \text{ g}^{-1} \text{ cm}^3$ , where  $\rho_{>} > \rho_*$  and  $\rho_{<} < \rho_*$  refer to the density in the high and low density region respectively. At the critical temperature  $T_c < T_*$  and pressure  $p_c < p_*$  for a first order transition one finds for the discontinuity in the density between the liquid ( $\rho_l$ ) and gas ( $\rho_g$ ) phase

$$\Delta\rho = \rho_l - \rho_g = B_p \left( \frac{p_* - p_c}{p_*} \right)^{\beta} = B_T \left( \frac{T_* - T_c}{T_*} \right)^{\beta} \tag{5.5}$$

with  $B_p = 0.85 \text{ g cm}^{-3}$ ,  $B_T = 1.5 \text{ g cm}^{-3}$ . This relation also defines the slope of the critical line near the endpoint.

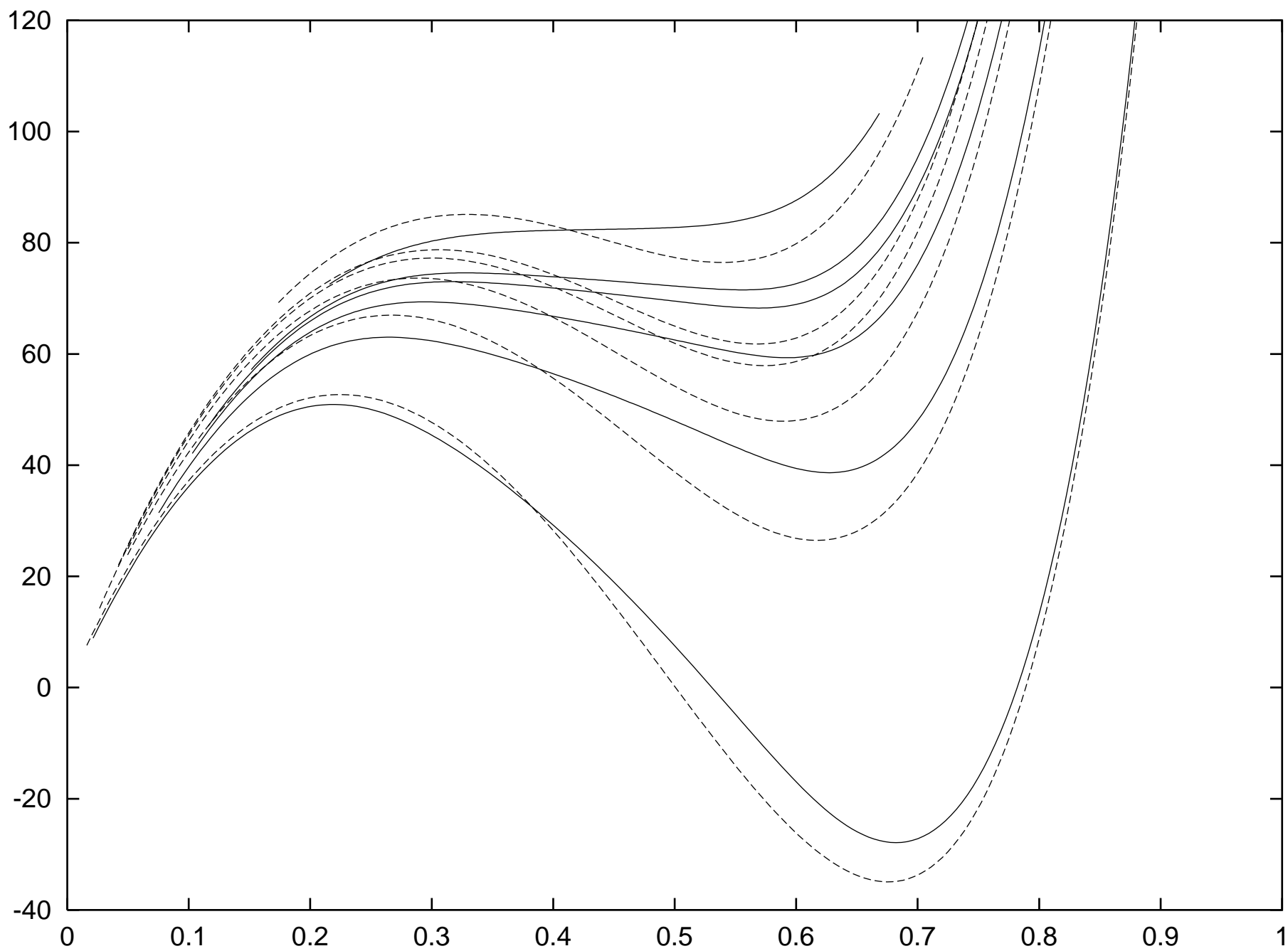
There is no apparent limitation for the use of the flow equation for an arbitrary microscopic free energy. This includes the case where  $U_{\Lambda}$  has several distinct minima and, in particular, the interesting case of a tricritical point. At present, the main inaccuracy arises from a simplification of the  $q^2$ -dependence of the four point function which reflects itself in an error in the anomalous dimension  $\eta$ . The simplification of the momentum dependence of the effective propagator in the flow equation plays presumably only a secondary role. In summary, the non-perturbative flow equation appears to be a very efficient tool for the establishment of an explicit quantitative connection between the microphysical interactions and the long-range properties of the free energy.

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Dim.beh. unren. Potential ( $k=0$ ) in Einheiten von  $\Lambda^{-1}$

